

Figure 1

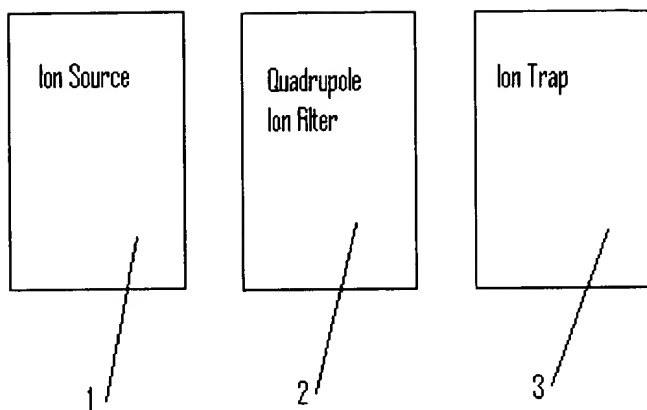


Figure 2

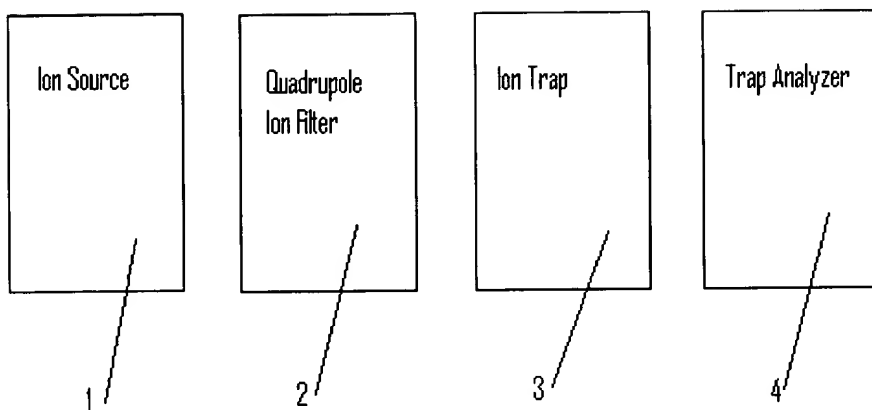


FIGURE 3

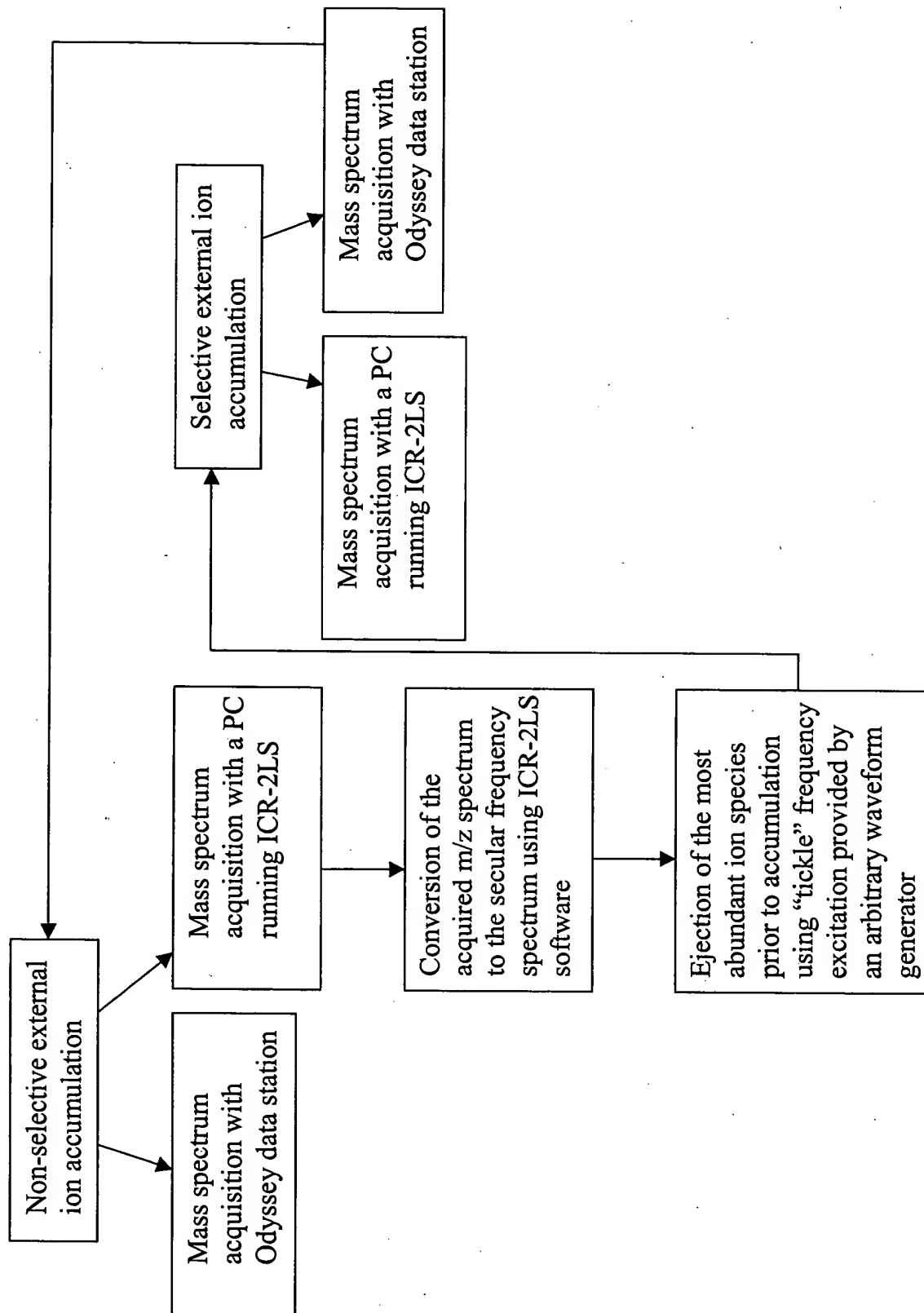


FIGURE 4

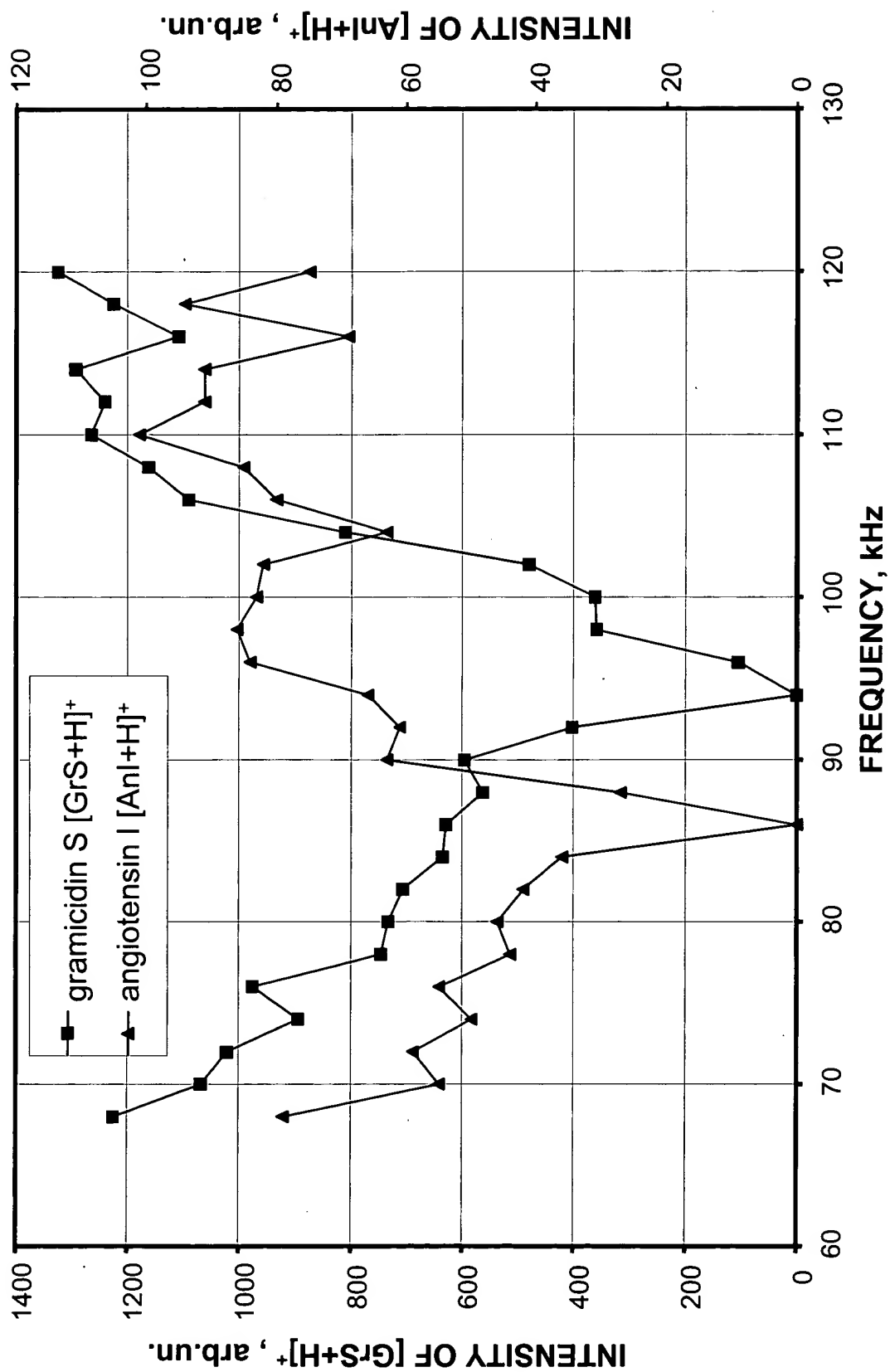


FIGURE 5

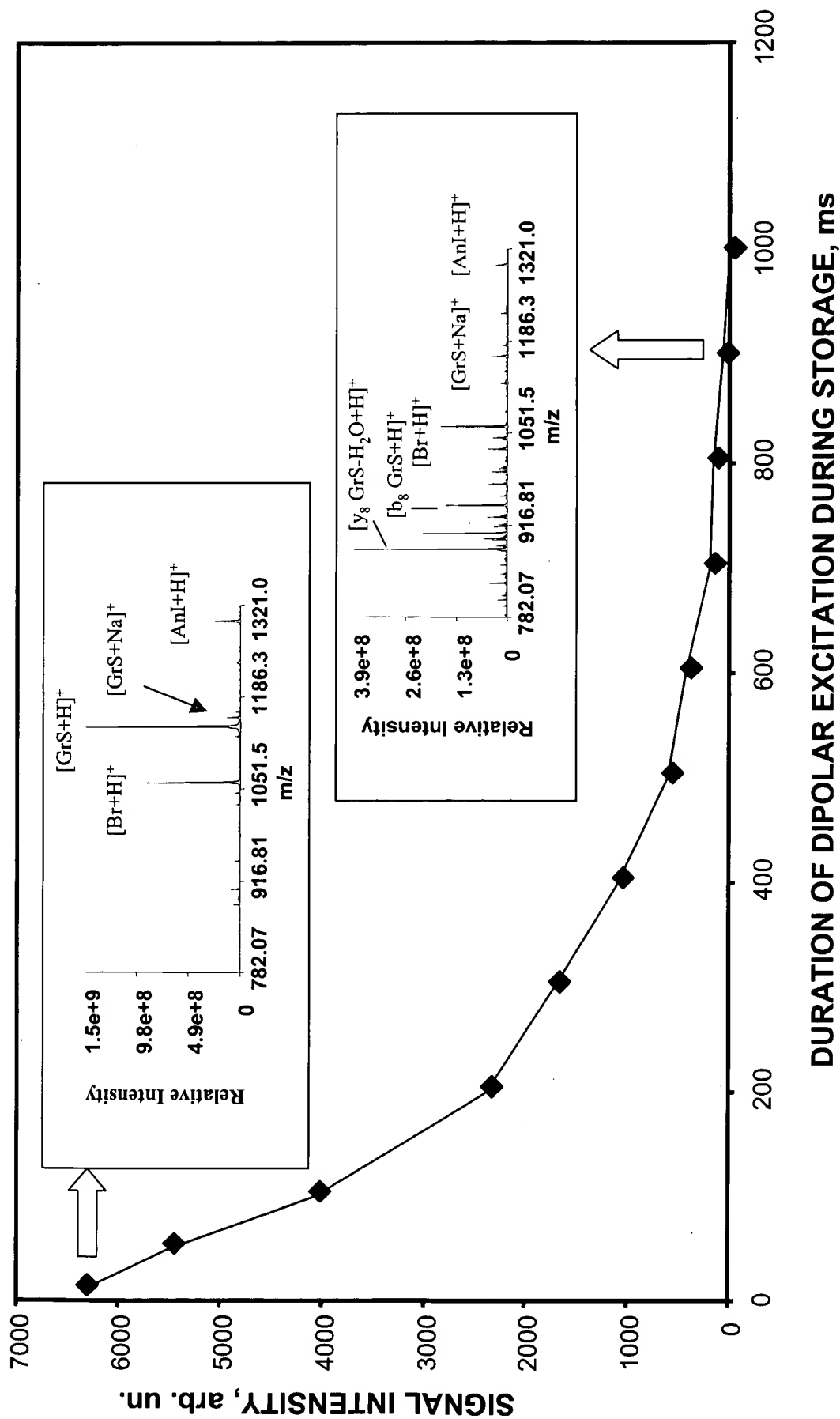


FIGURE 6

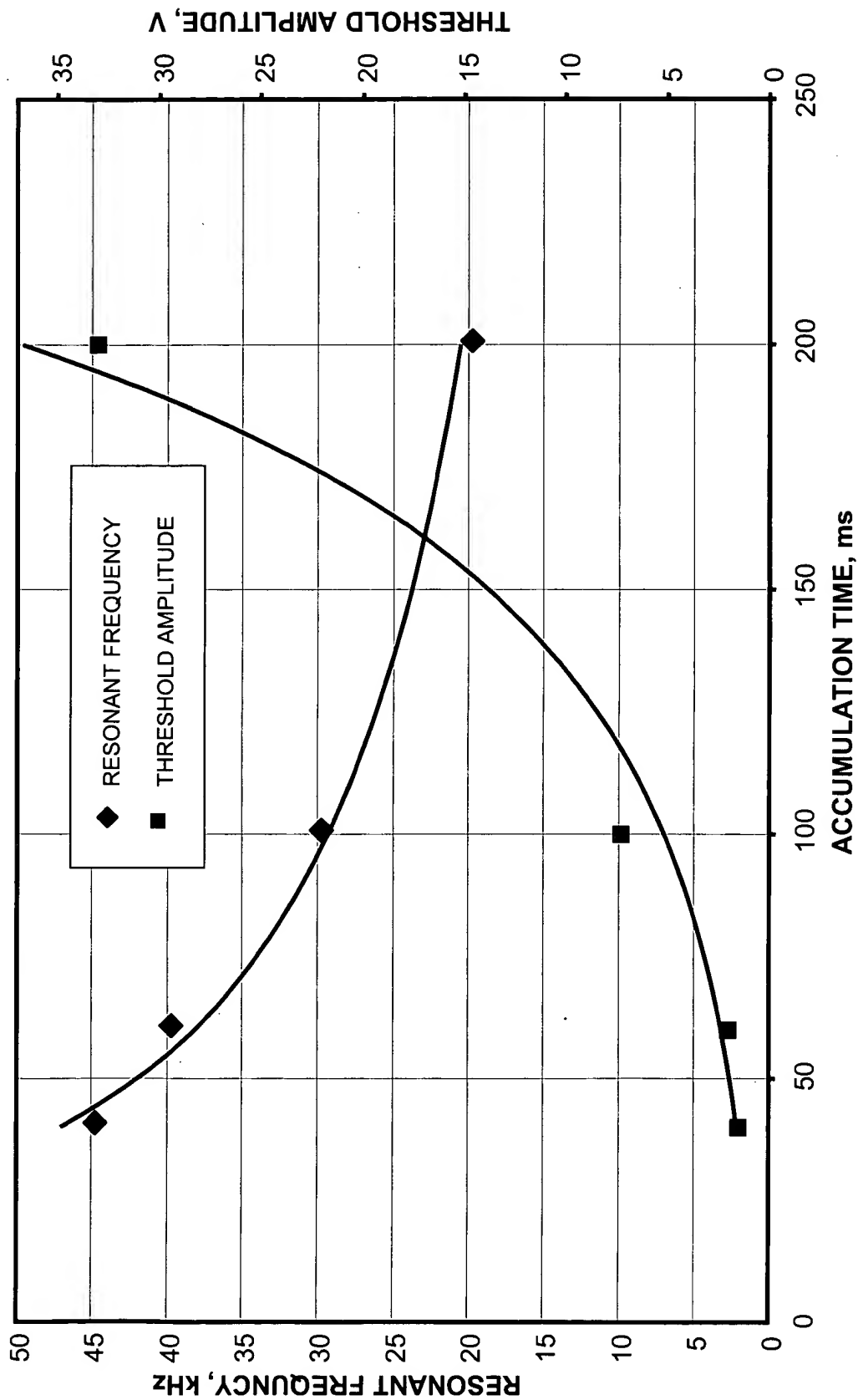


FIGURE 7

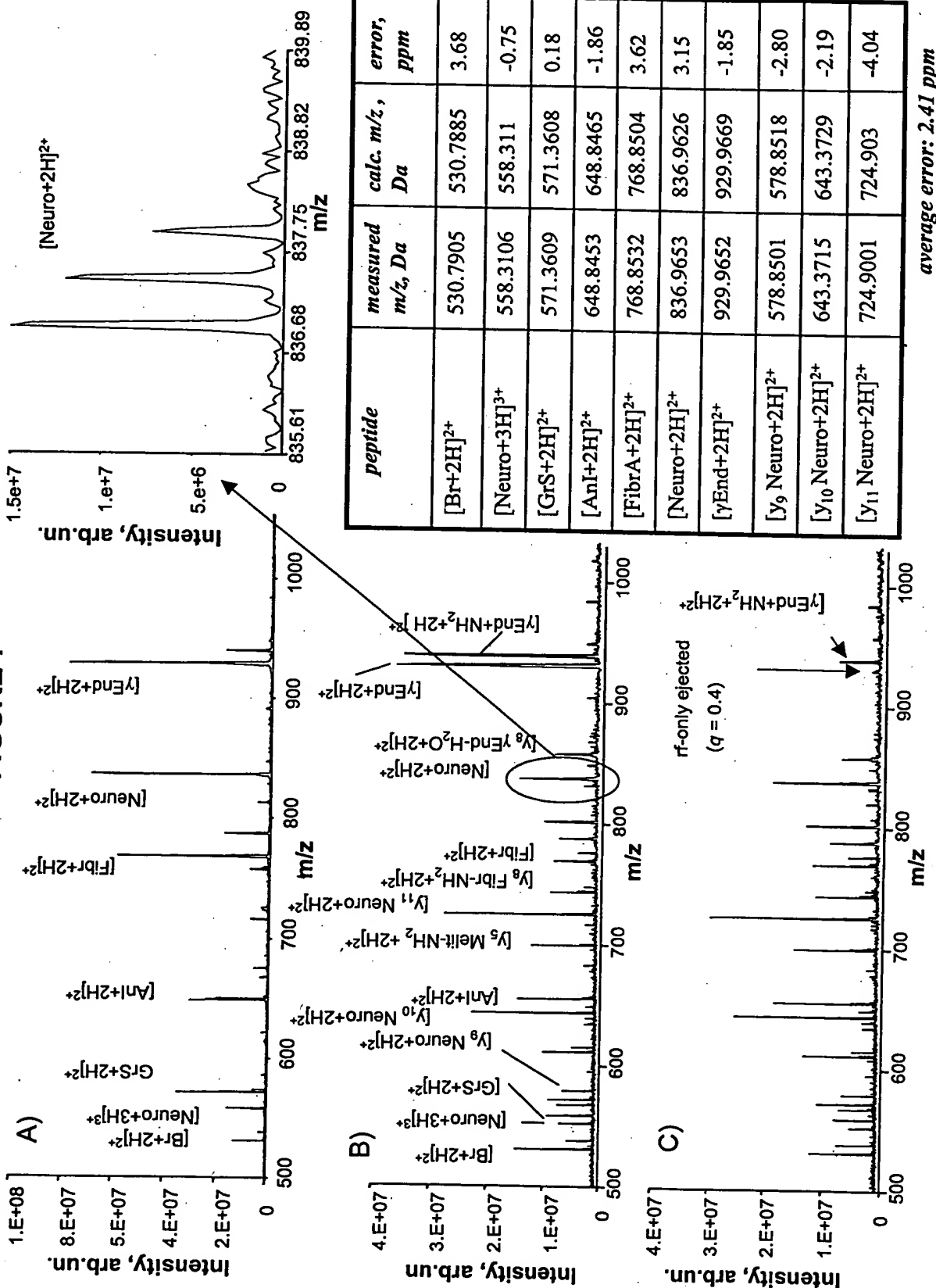
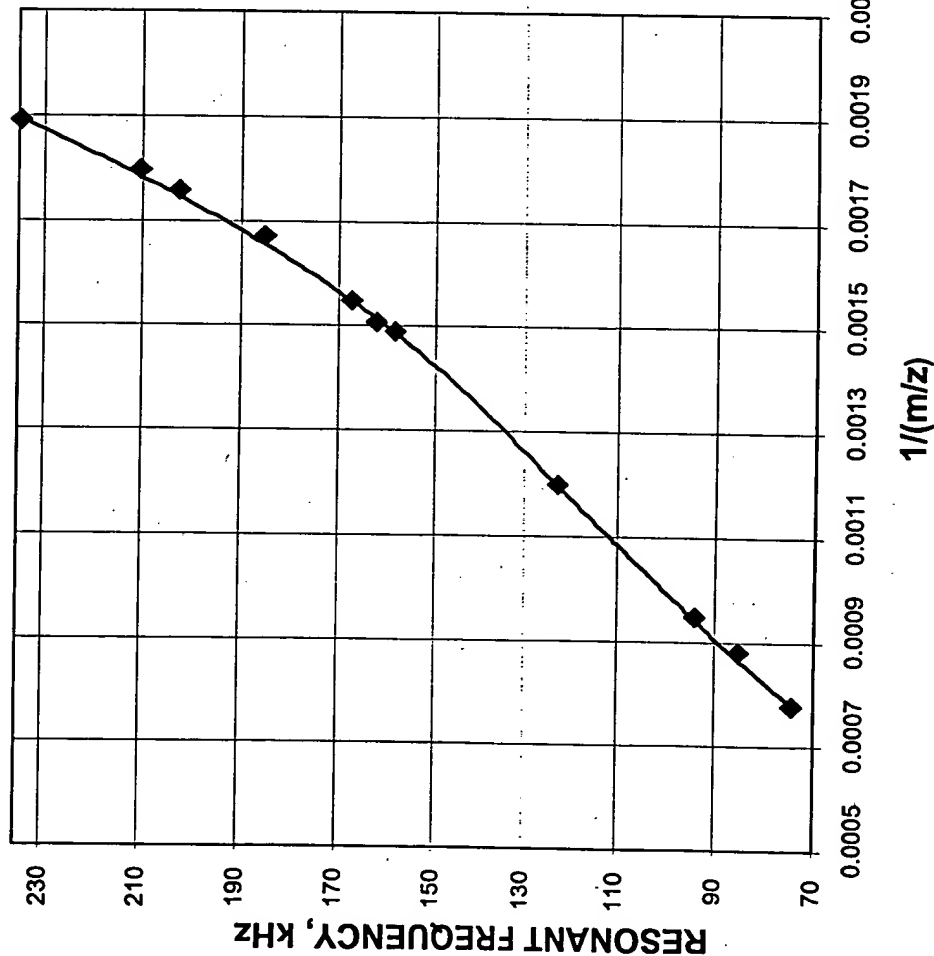


FIGURE 8

$$f_{\text{interpol}}(\text{Hz}) = 7.009470 \times 10^{13} \cdot x(1/m/z)^3 + 2.299154 \times 10^{11} \cdot x(1/m/z)^2 + 3.614403 \times 10^8 \cdot x(1/m/z) + 1.007772 \times 10^5$$



peptide	$f_{\text{exper}}(\text{Hz})$ , experiment	$f_{\text{predict}}(\text{Hz})$ , predicted	Maximum resolution
[Br+2H] <sup>2+</sup>	234500	232773.47	135
[Neuro+3H] <sup>3+</sup>	210500	211722.22	172
[GrS+2H] <sup>2+</sup>	202500	203511.93	200
[AnI+2H] <sup>2+</sup>	167500	166711.62	212
[SubP+2H] <sup>2+</sup>	158500	158145.75	447
[Neuro+2H] <sup>2+</sup>	122500	122390.09	1114
[Br+H] <sup>+</sup>	94000	94334.15	280
[GrS+H] <sup>+</sup>	85000	86457.77	58
[AngI+H] <sup>+</sup>	74500	73330.01	64



FIGURE 9

